CLAIMS

What is claimed is:

1. A method of characterizing spectrometer instruments according to instrumental variation, comprising the steps of:

providing standard spectral measurements from at least one spectrometer instrument; and

classifying said spectral measurements into predefined clusters on the basis of extracted spectral features; and

providing calibration models for each of said predefined clusters, wherein said calibration model compensates for said instrumental variation.

2. The method of Claim 1 wherein said instrumental variation comprises any of:

wavelength shifts;

nonlinear wavelength shifts;

wavelength expansions;

wavelength contractions;

nonlinear wavelength expansions;

source intensity drifts;

blackbody profile changes;

bandwidth changes;

resolution changes;

baseline deviations;

changes over time;

temperature effects;

detector response;

differences in optical components (e.g. long-pass filters or fiber optics);

variation related to mounting of references;

differences in the optical interface to the sample (fiber spacing);
linearity; and
detector cut-off.

3. The method of Claim 1, wherein said standard spectra are measured on a plurality of spectrometer instruments.

4. The method of Claim 1, wherein said standard spectral are measured on a single spectrometer instruments at successive time intervals.

5. The method of Claim 1, wherein said classifying step comprises the steps of:

extracting features; and

classifying said features according to a classification model and decision rule.

6. The method of Claim 5, wherein said feature extraction step comprises any mathematical transformation that enhances a particular aspect or quality of data that is useful for interpretation.

7. The method of Claim 3, wherein said classification model comprises means for determining a set of similarity measures with predefined classes.

8. The method of Claim 5, wherein said decision rule comprises means for assigning class membership on the basis of a set of measures calculated by a decision engine.

9. The method of Claim 4, wherein individual features are divided into two categories, said categories comprising:

abstract wherein said features are extracted using various computational methods ; and

simple features that are derived from an *a priori* understanding of a system, wherein said feature is directly related to an instrument parameter or component.

10. The method of Claim 7, wherein said abstract features are calculated using any of:

plotting primary principal components versus one another and identifying resulting clusters;

discrminant anlysis; and

k-means clustering.

11. The method of Claim 5, wherein said classification step further comprises the step of employing factor-based methods to build a model capable of representing variation in a measured spectrum related to variations in spectral response;

wherein projection of a measured absorbance spectrum onto said model constitutes a feature that represents spectral variation related to instrument variation.

12. The method of Claim 5, wherein said classifying step further comprises the steps of:

measuring the similarity of a feature to predefined clusters; and

assigning membership in a cluster.

13. The method of Claim 5, further comprising the step of:

assigning measurements in an exploratory data set to clusters.

14. The method of Claim 13, further comprising the step of:

using measurements and class assignments to determine a mapping from features to cluster assignments.

15. The method of Claim 13, further comprising the steps of:

defining clusters from said features in a supervised manner, wherein each set of features is divided into two or more regions, and wherein classes are defined by combinations of feature divisions;

designing a classifier subsequent to class definition through supervised pattern recognition by determining an optimal mapping or transformation from the feature space to a class estimate which minimizes the number of misclassifications; and

creating a model based on class definitions which transforms a measured set of features to an estimated classification.

16. The method of Claim 1, further comprising the step of providing calibration models for analysis of new sample measurements.

17. The method of Claim 16, wherein said calibration models model differences between said predefined clusters.

18. The method of Claim 16, wherein a master calibration model is developed for a first of said clusters from a set of exemplar spectra with reference values and pre-assigned classification definitions.

19. The method of Claim 18, further comprising the step of transferring said master calibration model to a plurality of slave calibration models, wherein a slave calibration model is calculated for each remaining cluster, and wherein a transform modifies said master calibration model to a slave calibration model in accordance with principal features defining each of said classes.

20. The method of Claim 19, wherein said transferring step comprises the steps of:

transferring said master calibration model to a first slave calibration model;

transferring said first slave calibration model to a second slave calibration model;

and repeating said transfer from one slave calibration model to another slave calibration model, until a calibration has been provided for each of said predefined clusters;

wherein a transform modifies said transferred calibration models in accordance with principal features defining each of said clusters.

21. The method of Claim 18, further comprising the step of transferring said master calibration model to a plurality of slave calibration models, wherein a slave calibration model is calculated for each remaining cluster, and wherein a transform modifies said slave calibration model to said master calibration model in accordance with principal features defining each of said classes.

22. The method of Claim 21, wherein said transferring step comprises the steps of:

transferring said master calibration model to a first slave calibration model;

transferring said first slave calibration model to a second slave calibration model;

and repeating said transfer from one slave calibration model to another slave calibration model, until a calibration has been provided for each of said predefined clusters;

wherein a transform modifies said transferred calibration models in accordance with principal features defining each of said clusters.

23. The method of Claim 16, wherein a different calibration model is developed for each class, and wherein said calibration models are developed

from a set of exemplar spectra, with reference values and pre-assigned cluster definitions.

24. The method of Claim 23, wherein a spectrum is assigned to one of many predefined clusters for which a calibration model has been developed.

25. The method of Claim 1, further comprising the steps of:

providing new spectral measurements;

comparing said new spectral measurements to each of said pre-defined clusters according to extracted spectral features;

reporting those measurements as outliers for which a matching cluster is not found.

26. A method of developing calibration models for spectral analysis comprising the steps of:

defining clusters from an exemplar data set of spectral measurements, wherein said clusters exhibit a high degree of internal similarity;

mapping said clusters to one another, wherein principal features distinguishing clusters from one another are determined;

calculating a calibration model for a first of said clusters, said calibration model comprising a master calibration;

transferring said master calibration to at least one slave calibration, wherein a slave calibration comprises a calibration derived by applying a transform to slave spectra such that the master calibration now models the difference between the master cluster and another cluster corresponding to said slave spectra.